Search	Most Recent Queries	Time Resu
<u>#52</u>	Search #49 and phosphinothricin	11:04:00
<u>#51</u>	Search #49 and sulfo*	11:03:39
<u>#50</u>	Search #49 and phosph*	11:03:29
<u>#49</u>	Search #48 and sulfoximine	11:03:15 <u>1</u> 4
<u>#48</u>	Related Articles for PubMed (Select 10224282)	11:02:24 <u>42</u>
<u>#46</u>	PubMed Citations for PubChem Substance (Select 638212)	11:02:10
<u>#45</u>	PubMed Citations for PubChem Substance (Select 638213)	11:02:02
<u>#44</u>	PubMed Citations for PubChem Substance (Select 638214)	11:01:57
<u>#40</u>	PubMed Citations for PubChem Substance (Select 638211)	11:00:04
<u>#33</u>	PubMed Citations for PubChem Compound (Select 480050)	10:56:31
<u>#32</u>	PubMed Citations for PubChem Substance (Select 638215)	10:56:17
<u>#23</u>	Related Articles for PubMed (Select 6113985)	10:53:33 <u>12</u>
<u>#22</u>	Search Experientia[Jour] AND 461[page] AND 1981[pdat]	10:49:48
<u>#21</u>	Search "Lejczak B"[Author]	10:48:31

=> fil reg FILE 'REGISTRY' ENTERED AT 08:56:51 ON 20 JUL 2006 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2006 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 18 JUL 2006 HIGHEST RN 894196-03-3 DICTIONARY FILE UPDATES: 18 JUL 2006 HIGHEST RN 894196-03-3

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 6, 2006

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

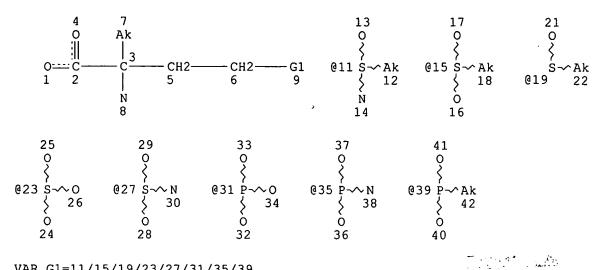
VAR G1=S/P NODE ATTRIBUTES: DEFAULT MLEVEL IS ATOM DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES: RING(S) ARE ISOLATED OR EMBEDDED NUMBER OF NODES IS 9

STEREO ATTRIBUTES: NONE

L3 311 SEA FILE=REGISTRY SSS FUL L1

L6 STR



VAR G1=11/15/19/23/27/31/35/39

NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 40

STEREO ATTRIBUTES: NONE

28 SEA FILE=REGISTRY SUB=L3 CSS FUL L6 L8

100.0% PROCESSED 113 ITERATIONS 28 ANSWERS

SEARCH TIME: 00.00.03

=> d ide can tot 18

L8 ANSWER 1 OF 28 REGISTRY COPYRIGHT 2006 ACS on STN

858741-14-7 REGISTRY RN

Entered STN: 07 Aug 2005 ED

CN INDEX NAME NOT YET ASSIGNED

FS 3D CONCORD

MF C7 H16 N O5 P

Chemical Library SR

Supplier: Aurora Fine Chemicals

LC STN Files: CHEMCATS

$$\begin{array}{c|c} & \text{NH}_2 \\ | & \\ \text{i-Pr-C-CH}_2\text{--CH}_2\text{--PO}_3\text{H}_2 \\ | & \\ \text{CO}_2\text{H} \end{array}$$

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

ANSWER 2 OF 28 REGISTRY COPYRIGHT 2006 ACS on STN  $^{18}$ 

RN 844864-14-8 REGISTRY

ED Entered STN: 10 Mar 2005

CN L-Isovaline, 4-phosphono-, hydrochloride (9CI) (CA INDEX NAME)

OTHER NAMES:

(S)-2-Amino-2-methyl-4-phosphonobutanoic acid hydrochloride CN

STEREOSEARCH FS

C5 H12 N O5 P . C1 H MF

SR

LC STN Files: CA, CAPLUS, CASREACT, CHEMCATS

CRN (157381-42-5)

Absolute stereochemistry. Rotation (+).

#### HC1

#### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 142:240508

rsANSWER 3 OF 28 REGISTRY COPYRIGHT 2006 ACS on STN

RN 743387-50-0 REGISTRY

ED Entered STN: 12 Sep 2004

CN Butanoic acid, 2-amino-2-ethyl-4-(hydroxymethylphosphinyl)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C7 H16 N O4 P

CI COM

SR CA

### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

rsANSWER 4 OF 28 REGISTRY COPYRIGHT 2006 ACS on STN

258284-99-0 REGISTRY RN

Entered STN: 06 Mar 2000

CN L-Valine, 2-(2-phosphonoethyl)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

C7 H16 N O5 P

SR CA

LC STN Files: CA, CAPLUS

Absolute stereochemistry.

#### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 132:151895

L8 ANSWER 5 OF 28 REGISTRY COPYRIGHT 2006 ACS on STN

RN 220288-10-8 REGISTRY

ED Entered STN: 09 Mar 1999

CN Isovaline, 4-(hydroxymethylphosphinyl)-, ammonium salt (9CI) (CA INDEX NAME)

MF C6 H14 N O4 P . x H3 N

SR CA

LC STN Files: CA, CAPLUS, CASREACT, USPATFULL

CRN (65482-86-2)

$$\begin{array}{c|c} & \text{NH2} & \text{O} \\ & \text{HO}_2\text{C} - \text{C} - \text{CH}_2 - \text{CH}_2 - \text{P} - \text{Me} \\ & \text{Me} & \text{OH} \end{array}$$

## •x NH3

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 130:153794

L8 ANSWER 6 OF 28 REGISTRY COPYRIGHT 2006 ACS on STN

RN 204438-84-6 REGISTRY

ED Entered STN: 23 Apr 1998

CN Butanoic acid, 2-amino-4-(S-butylsulfonimidoyl)-2-ethyl- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C10 H22 N2 O3 S

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 128:213410

L8 ANSWER 7 OF 28 REGISTRY COPYRIGHT 2006 ACS on STN

RN 204438-79-9 REGISTRY

ED Entered STN: 23 Apr 1998

CN Butanoic acid, 2-amino-4-(S-butylsulfonimidoyl)-2-ethyl-, [S-(R\*,R\*)]-(9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C10 H22 N2 O3 S

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL

Absolute stereochemistry.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 128:213410

L8 ANSWER 8 OF 28 REGISTRY COPYRIGHT 2006 ACS on STN

RN 171483-43-5 REGISTRY

ED Entered STN: 19 Dec 1995

CN D-Isovaline, 4-phosphono- (9CI) (CA INDEX NAME)

OTHER NAMES:

CN (R)-2-Amino-2-methyl-4-phosphonobutanoic acid

FS STEREOSEARCH

MF C5 H12 N O5 P

SR CA

LC STN Files: CA, CAPLUS, CASREACT, CHEMCATS

Absolute stereochemistry. Rotation (-).

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 142:240508

REFERENCE 2: 124:30404

L8 ANSWER 9 OF 28 REGISTRY COPYRIGHT 2006 ACS on STN

RN 171228-34-5 REGISTRY

ED Entered STN: 12 Dec 1995

CN L-Isovaline, 4-sulfo- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C5 H11 N O5 S

SR CA

LC STN Files: CA, CAPLUS

Absolute stereochemistry.

### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 136:318765 224

REFERENCE 2: 124:30404

L8 ANSWER 10 OF 28 REGISTRY COPYRIGHT 2006 ACS on STN

RN 170984-73-3 REGISTRY

ED Entered STN: 06 Dec 1995

CN Butanoic acid, 2-amino-2-ethyl-4-phosphono-, (S)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C6 H14 N O5 P

SR CA

LC STN Files: CA, CAPLUS

Absolute stereochemistry.

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 124:30404

L8 ANSWER 11 OF 28 REGISTRY COPYRIGHT 2006 ACS on STN

RN 157381-42-5 REGISTRY

ED Entered STN: 01 Sep 1994

CN L-Isovaline, 4-phosphono- (9CI) (CA INDEX NAME)

OTHER NAMES:

CN  $\alpha$ -Methyl-L-AP 4

CN 4-Phosphono-L-isovaline

FS STEREOSEARCH

DR 181361-62-6

MF C5 H12 N O5 P

CI COM

SR CA

LC STN Files: CA, CAPLUS, CASREACT, CHEMCATS, CSCHEM, TOXCENTER, USPAT2, USPATFULL

.

Absolute stereochemistry. Rotation (+).

#### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

- 39 REFERENCES IN FILE CA (1907 TO DATE)
  - 2 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
  - 39 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 142:85952

REFERENCE 2: 140:23256

REFERENCE 3: 140:22628

REFERENCE 4: 138:130580

REFERENCE 5: 137:363255

REFERENCE 6: 136:318765

REFERENCE 7: 135:376738

REFERENCE 8: 135:352635

REFERENCE 9: 135:55950

REFERENCE 10: 134:193694

L8 ANSWER 12 OF 28 REGISTRY COPYRIGHT 2006 ACS on STN

RN 155330-54-4 REGISTRY

ED Entered STN: 26 May 1994

CN Isovaline, 4-sulfo- (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN DL-Isovaline, 4-sulfo-

FS 3D CONCORD

MF C5 H11 N O5 S

SR CA

LC STN Files: CA, CAPLUS

#### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 121:9939

L8 ANSWER 13 OF 28 REGISTRY COPYRIGHT 2006 ACS on STN

RN 141609-98-5 REGISTRY

ED Entered STN: 05 Jun 1992

CN L-Isovaline, 4-(hydroxymethylphosphinyl)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C6 H14 N O4 P

SR CA

LC STN Files: BEILSTEIN\*, CA, CAPLUS

(\*File contains numerically searchable property data)

Absolute stereochemistry.

## \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 117:106229

L8 ANSWER 14 OF 28 REGISTRY COPYRIGHT 2006 ACS on STN

RN 115730-43-3 REGISTRY

ED Entered STN: 13 Aug 1988

CN Isovaline, 4-(hydroxymethylphosphinyl)-, monoammonium salt (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN DL-Isovaline, 4-(hydroxymethylphosphinyl)-, monoammonium salt

MF C6 H14 N O4 P . H3 N

SR CA

LC STN Files: BEILSTEIN\*, CA, CAPLUS, CASREACT

(\*File contains numerically searchable property data)

CRN (65482-86-2)

# ● NH3

3 REFERENCES IN FILE CA (1907 TO DATE)

3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 112:32528

REFERENCE 2: 110:150325

REFERENCE 3: 109:110882

L8 ANSWER 15 OF 28 REGISTRY COPYRIGHT 2006 ACS on STN

RN 115651-45-1 REGISTRY

ED Entered STN: 06 Aug 1988

CN Butanoic acid, 2-amino-2-ethyl-4-(hydroxymethylphosphinyl)-, monosodium

salt (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN Butanoic acid, 2-amino-2-ethyl-4-(hydroxymethylphosphinyl)-, monosodium

salt,  $(\pm)$ -

MF C7 H16 N O4 P . Na

SR CA

LC STN Files: BEILSTEIN\*, CA, CAPLUS, CASREACT

(\*File contains numerically searchable property data)

CRN (743387-50-0) : :

#### Na

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 109:110882

L8 ANSWER 16 OF 28 REGISTRY COPYRIGHT 2006 ACS on STN

RN 104739-23-3 REGISTRY

ED Entered STN: 18 Oct 1986

CN 4-Pentenoic acid, 2-amino-2-(2-phosphonoethyl)-, (S)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C7 H14 N O5 P

SR CA

LC STN Files: BEILSTEIN\*, CA, CAPLUS, CASREACT (\*File contains numerically searchable property data)

#### Absolute stereochemistry.

#### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 106:5390

L8 ANSWER 17 OF 28 REGISTRY COPYRIGHT 2006 ACS on STN

RN 95833-68-4 REGISTRY

ED Entered STN: 13 Apr 1985

CN D-Isovaline, 4-(methylsulfonyl)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C6 H13 N O4 S

LC STN Files: BEILSTEIN\*, CA, CAPLUS

(\*File contains numerically searchable property data)

#### Absolute stereochemistry.

## \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

### REFERENCE 1: 102:178450

L8 ANSWER 18 OF 28 REGISTRY COPYRIGHT 2006 ACS on STN

RN 95833-67-3 REGISTRY

ED Entered STN: 13 Apr 1985

CN L-Isovaline, 4-(methylsulfonyl)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C6 H13 N O4 S

LC STN Files: BEILSTEIN\*, CA, CAPLUS

(\*File contains numerically searchable property data)

Absolute stereochemistry.

#### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 102:178450

REFERENCE 2: 50:73727

L8 ANSWER 19 OF 28 REGISTRY COPYRIGHT 2006 ACS on STN

RN 95833-66-2 REGISTRY

ED Entered STN: 13 Apr 1985

CN D-Isovaline, 4-(methylsulfinyl)-, (S)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C6 H13 N O3 S

LC STN Files: BEILSTEIN\*, CA, CAPLUS

(\*File contains numerically searchable property data)

Absolute stereochemistry.

## \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 102:178450

L8 ANSWER 20 OF 28 REGISTRY COPYRIGHT 2006 ACS on STN

RN 95833-65-1 REGISTRY

ED Entered STN: 13 Apr 1985

CN D-Isovaline, 4-(methylsulfinyl)-, (R)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C6 H13 N O3 S

LC STN Files: BEILSTEIN\*, CA, CAPLUS

(\*File contains numerically searchable property data)

Absolute stereochemistry.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 102:178450

L8 ANSWER 21 OF 28 REGISTRY COPYRIGHT 2006 ACS on STN

RN 95833-64-0 REGISTRY

ED Entered STN: 13 Apr 1985

CN L-Isovaline, 4-(methylsulfinyl)-, (S)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C6 H13 N O3 S

LC STN Files: BEILSTEIN\*, CA, CAPLUS

(\*File contains numerically searchable property data)

Absolute stereochemistry.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 102:178450

L8 ANSWER 22 OF 28 REGISTRY COPYRIGHT 2006 ACS on STN

RN 95833-63-9 REGISTRY

ED Entered STN: 13 Apr 1985

CN L-Isovaline, 4-(methylsulfinyl)-, (R)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C6 H13 N O3 S

LC STN Files: BEILSTEIN\*, CA, CAPLUS

(\*File contains numerically searchable property data)

Absolute stereochemistry.

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 102:178450

L8 ANSWER 23 OF 28 REGISTRY COPYRIGHT 2006 ACS on STN

RN 78405-44-4 REGISTRY

ED Entered STN: 16 Nov 1984

CN Isovaline, 4-phosphono- (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN DL-Isovaline, 4-phosphono-

OTHER NAMES:

CN 2-Amino-2-methyl-4-phosphonobutanoic acid

DR 75787-84-7

MF C5 H12 N O5 P

LC STN Files: BEILSTEIN\*, CA, CAPLUS, CASREACT, CHEMCATS, TOXCENTER (\*File contains numerically searchable property data)

$$H_2N$$
 $H_2C$ 
 $PO_3H_2$ 

#### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

7 REFERENCES IN FILE CA (1907 TO DATE)

7 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 142:240508

REFERENCE 2: 133:69122

REFERENCE 3: 117:184255

REFERENCE 4: 102:198188

REFERENCE 5: 102:197823

REFERENCE 6: 95:57044

REFERENCE 7: 94:140

L8 ANSWER 24 OF 28 REGISTRY COPYRIGHT 2006 ACS on STN

RN 70056-05-2 REGISTRY

ED Entered STN: 16 Nov 1984

CN Isovaline, 4-(S-propylsulfonimidoyl)- (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN DL-Isovaline, 4-(S-propylsulfonimidoyl)-

OTHER NAMES:

CN  $\alpha$ -Methyl-DL-prothionine-SR-sulfoximine

MF C8 H18 N2 O3 S

LC STN Files: CA, CAPLUS

#### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 90:198299

L8 ANSWER 25 OF 28 REGISTRY COPYRIGHT 2006 ACS on STN

RN 70056-03-0 REGISTRY

ED Entered STN: 16 Nov 1984

CN Isovaline, 4-(S-ethylsulfonimidoyl)- (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN DL-Isovaline, 4-(S-ethylsulfonimidoyl)-

MF C7 H16 N2 O3 S

LC STN Files: CA, CAPLUS

## \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 90:198299

L8 ANSWER 26 OF 28 REGISTRY COPYRIGHT 2006 ACS on STN

RN 66735-68-0 REGISTRY

ED Entered STN: 16 Nov 1984

CN Butanoic acid, 2-amino-2-ethyl-4-(S-methylsulfonimidoyl)- (9CI) (CA INDEX NAME)

OTHER NAMES:

CN α-Ethyl-DL-methionine-SR-sulfoximine

FS 3D CONCORD

DR 113282-47-6

and the second

MF C7 H16 N2 O3 S

LC STN Files: CA, CAPLUS, MEDLINE, TOXCENTER, USPATFULL

### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

mampagarang an has

4 REFERENCES IN FILE CA (1907 TO DATE)

4 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 141:12262

REFERENCE 2: 108:132274

REFERENCE 3: 90:198299

REFERENCE 4: 89:100916

L8 ANSWER 27 OF 28 REGISTRY COPYRIGHT 2006 ACS on STN

RN 66735-67-9 REGISTRY

ED Entered STN: 16 Nov 1984

CN Isovaline, 4-(S-methylsulfonimidoyl)- (9CI) (CA INDEX NAME)

OTHER NAMES:

CN  $\alpha$ -Methyl-DL-methionine (SR)-sulfoximine

FS 3D CONCORD

MF C6 H14 N2 O3 S

LC STN Files: BEILSTEIN\*, CA, CAPLUS, TOXCENTER, USPATFULL (\*File contains numerically searchable property data)

## \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

5 REFERENCES IN FILE CA (1907 TO DATE)

5 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 141:12262

REFERENCE 2: 114:38443

REFERENCE 3: 90:198299

REFERENCE 4: 89:100916

REFERENCE 5: 50:73727

L8 ANSWER 28 OF 28 REGISTRY COPYRIGHT 2006 ACS on STN

65482-86-2 REGISTRY RN

Entered STN: 16 Nov 1984 ED

CN Isovaline, 4-(hydroxymethylphosphinyl)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

DR 78405-45-5

MF C6 H14 N O4 P

CI COM

BEILSTEIN\*, CA, CAPLUS, IFICDB, IFIPAT, IFIUDB, TOXCENTER, LC STN Files: USPATFULL

(\*File contains numerically searchable property data)

#### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

6 REFERENCES IN FILE CA (1907 TO DATE)

6 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 104:218953

REFERENCE 2: 95:57044

REFERENCE 94:151895 3:

REFERENCE 93:8479 4:

REFERENCE 89:141899 5:

REFERENCE 6: 88:70494

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(FILE 'REGISTRY' ENTERED AT 08:43:50 ON 20 JUL 2006)

L8 28 S L6 CSS FUL SUB=L3

SAV L8 ISSAC715A/A

FILE 'HCAOLD' ENTERED AT 08:48:16 ON 20 JUL 2006

L9 0 S L8

FILE 'HCAPLUS' ENTERED AT 08:48:21 ON 20 JUL 2006

L10 66 S L8

L11 1 S US20040157802/PN OR (US2003-715679# OR WO2003-US36705 OR US20

E HORWITZ M/AU

L12 128 S E3-E6, E12, E13

E HARTH G/AU

L13 54 S E3, E4, E7, E8

E GRIFFITH O/AU

176 S E3, E16, E21, E24 L14

L15 5 S L10 AND L11-L14

FILE 'REGISTRY' ENTERED AT 08:50:50 ON 20 JUL 2006

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L16
              1 S 9023-70-5
     FILE 'HCAPLUS' ENTERED AT 08:51:55 ON 20 JUL 2006
           6221 S L16
L17
L18
           7476 S GLUTAMINE() (SYNTHETASE OR SYNTHASE)
L19
             67 S GLUTAMATE() (AMMONIA LIGASE OR ETHYLAMINE LIGASE)
L20
              O S GLUTAMYLHYDROXAMIC () (SYNTHETASE OR SYNTHASE)
              7 S L10 AND L17-L19
L21
L22
              9 S L15, L21
             11 S L8(L) (THU OR PAC OR PKT OR DMA)/RL
L23
L24
             29 S L10 AND (PHARMACEUT? OR PHARMACOL? OR BIOMOL? OR PATHOL?)/SC,
             64 S L10 AND (PY<=2002 OR PRY<=2002 OR AY<=2002)
L25
L26
              9 S L22 AND L25
L27
             10 S L23 AND L25
L28
             28 S L24 AND L25
                E MYCOBACTERIUM/CT
          27923 S E3+OLD, NT
L29
L30
              1 S L29 AND L25
L31
              9 S L26, L30
L32
              2 S L27, L28 AND L31
L33
              9 S L31, L32
L34
             26 S L27, L28 NOT L33
     FILE 'REGISTRY' ENTERED AT 08:56:51 ON 20 JUL 2006
=> d ide can 116
L16 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2006 ACS on STN
     9023-70-5 REGISTRY
ED
     Entered STN: 16 Nov 1984
     Synthetase, glutamine (9CI) (CA INDEX NAME)
OTHER NAMES:
     E.C. 6.3.1.2
CN
     Glutamate ammonia ligase
CN
     Glutamate-ethylamine ligase
CN
     Glutamine synthase
CN
     Glutamine synthetase
CN
     Glutamylhydroxamic synthetase
CN
     L-Glutamine synthetase
MF
     Unspecified
CI
     MAN
LC
     STN Files:
                  AGRICOLA, ANABSTR, BIOSIS, BIOTECHNO, CA, CABA, CAPLUS,
       CASREACT, CBNB, CHEMINFORMRX, CIN, CSCHEM, CSNB, EMBASE, IFICDB, IFIPAT,
       IFIUDB, IPA, PROMT, TOXCENTER, USPAT2, USPATFULL
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**
            6215 REFERENCES IN FILE CA (1907 TO DATE)
              59 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
            6220 REFERENCES IN FILE CAPLUS (1907 TO DATE)
REFERENCE
            1: 145:61696
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jan delaval - 20 july 2006

REFERENCE

REFERENCE

REFERENCE

2:

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REFERENCE 10: 145:40851

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FILE COVERS 1907 - 20 Jul 2006 VOL 145 ISS 4 FILE LAST UPDATED: 19 Jul 2006 (20060719/ED)

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L33 ANSWER 1 OF 9 HCAPLUS COPYRIGHT 2006 ACS on STN

AN 2004:452975 HCAPLUS

DN 141:12262

ED Entered STN: 04 Jun 2004

- TI Anti-microbial agents derived from methionine sulfoximine analogues and use for treating mycobacterial infections
- IN Harth, Gunter; Griffith, Owen W.; Horwitz, Marcus
- PA Regents of the University of California, USA
- SO PCT Int. Appl., 40 pp.

CODEN: PIXXD2

DT Patent

LA English

IC ICM A61K

CC 63-5 (Pharmaceuticals)

FAN.CNT 1

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OS
     MARPAT 141:12262
     Novel antimicrobial compns. containing analogs of L-methionine-SR-sulfóximine
·AB
     (MSO) that are effective in treating intracellular pathogen infections are
                Specifically, the compns. provided are MSO analogs having
     superior antimicrobial activity with significantly less toxicity as
     compared to MSO. These MSO analogs are suitable for use in treating
     infection in animals including primates, cows, pigs, horses, rabbits,
     mice, rats, cats, and dogs. Moreover, the MSO analogs are ideally suited
     for treating infections caused by the genus Mycobacterium. Addnl.,
     methods for using the novel MSO analogs are also provided.
ST
     antimicrobial agent mycobacterium methionine sulfoximine analog
IT
     Bos taurus
     Canis familiaris
     Equus caballus
     Felis catus
     Human
     Mammalia
     Monkey
       Mycobacterium avium
       Mycobacterium bovis
```

Mycobacterium tuberculosis

Oryctolagus cuniculus

Rodentia

Sus scrofa domestica

(anti-microbial agents derived from methionine sulfoximine analogs and use for treating mycobacterial infections)

IT Antibacterial agents

(anti-mycobacterial; anti-microbial agents derived from methionine sulfoximine analogs and use for treating mycobacterial infections)

IT Infection

(bacterial, mycobacterial, treatment of; anti-microbial agents derived from methionine sulfoximine analogs and use for treating mycobacterial infections)

IT Mycobacterium

(infection, treatment of; anti-microbial agents derived from methionine sulfoximine analogs and use for treating mycobacterial infections)

IT 7732-18-5, Water, uses

RL: NUU (Other use, unclassified); USES (Uses)

(anti-microbial agents derived from methionine sulfoximine analogs and use for treating mycobacterial infections)

IT 74-93-1, Methane thiol, reactions 143-33-9, Sodium cyanide 1066-33-7,
 Ammonium bicarbonate 1629-58-9, Ethyl vinyl ketone 5925-75-7
 26628-22-8, Sodium azide

RL: RCT (Reactant); RACT (Reactant or reagent)

(anti-microbial agents derived from methionine sulfoximine analogs and use for treating mycobacterial infections)

IT 66735-71-5P,  $\alpha$ -Ethyl-DL-methionine

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(anti-microbial agents derived from methionine sulfoximine analogs and use for treating mycobacterial infections)

IT 50-81-7, Ascorbic acid, biological studies 54-85-3, Isoniazid 1982-67-8D, Methionine sulfoximine, analogs 15985-39-4 66735-67-9 66735-68-0

RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses) (anti-microbial agents derived from methionine sulfoximine analogs and use for treating mycobacterial infections)

IT 9023-70-5, Glutamine synthetase (

RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses) (inhibitor; anti-microbial agents derived from methionine sulfoximine analogs and use for treating mycobacterial infections)

IT 66735-67-9 66735-68-0

RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses) (anti-microbial agents derived from methionine sulfoximine analogs and use for treating mycobacterial infections)

RN 66735-67-9 HCAPLUS

CN Isovaline, 4-(S-methylsulfonimidoyl)- (9CI) (CA INDEX NAME)

RN 66735-68-0 HCAPLUS

CN Butanoic acid, 2-amino-2-ethyl-4-(S-methylsulfonimidoyl)- (9CI) (CA INDEX NAME)

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ΙT
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        (inhibitor; anti-microbial agents derived from methionine sulfoximine
        analogs and use for treating mycobacterial infections)
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CN
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     Stamler, Jonathan S.; Griffith, Owen W.
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     CODEN: PIXXD2
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AB
     Mammals are treated for infections or for conditions associated with pathol.
     proliferating mammalian cell growth (for example, certain cancers,
     restenosis, benign prostatic hypertrophy) by administration of a
     manipulator of nitrosative stress to selectively kill or reduce the growth
     of the microbes or helminths causing the infection or of host cells
     infected with the microbes or of the pathol. proliferating mammalian
     cells. Novel agents include \alpha-alkyl-S-alkyl-homocysteine
     sulfoximines wherein the \alpha-alkyl contains 2-8 carbon atoms, and the
     S-alkyl contains 1-10 carbon atoms. In another invention herein, mammals
     in need of increased nitrosative stress defenses are treated, e.g. humans
     at risk for a stroke because of having had a transient ischemic attack are
     treated. Treatments to increase nitrosative stress defenses include, for
     example, repeated administrations of low doses of manipulators of
     nitrosative stress so that the subject treated has increased tolerance to
     nitrosative stress. In still another invention, mammals are treated for
     protozoal infections by systemic administration of L-buthionine-S-
     sulfoximine and agent that increases nitrosative stress.
ST
     nitrosative oxidative stress modulator therapeutic; alkylhomocysteine
```

sulfoximine nitrosative stress therapeutic; ethylbuthionine sulfoximine prepn nitrosative stress therapeutic; buthionine sulfoximine protozoal infection

IT Promoter (genetic element)
 mRNA

RL: BSU (Biological study, unclassified); BIOL (Biological study) (OxyR, antisense construct to; nitrosative and oxidative stress modulators for the treatment of disease)

IT Thiols (organic), biological studies

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(S-nitroso; nitrosative and oxidative stress modulators for the treatment of disease)

IT Tripeptides

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(S-nitrosocysteine-containing; nitrosative and oxidative stress modulators for the treatment of disease)

IT Thiols (organic), biological studies

RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)

(and mycothiols and ovothiols; nitrosative and oxidative stress modulators for the treatment of disease)

IT Artery

100 4 300

(angioplasty; nitrosative and oxidative stress modulators for the treatment of disease)

IT Proteins, specific or class

RL: BSU (Biological study, unclassified); BIOL (Biological study) (anti-nitrosative stress gene products; nitrosative and oxidative stress modulators for the treatment of disease)

IT Gene

RL: BSU (Biological study, unclassified); BIOL (Biological study) (anti-nitrosative stress; nitrosative and oxidative stress modulators for the treatment of disease)

IT Nucleic acids

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(antisense constructs; nitrosative and oxidative stress modulators for the treatment of disease)

IT Prostate gland

(benign hyperplasia; nitrosative and oxidative stress modulators for the treatment of disease)

IT Candida albicans

(candidiasis from, oral; nitrosative and oxidative stress modulators for the treatment of disease)

IT Antitumor agents

(carcinoma, genitourinary; nitrosative and oxidative stress modulators for the treatment of disease)

IT Head

Head

Neck, anatomical

Neck, anatomical

(carcinoma, inhibitors; nitrosative and oxidative stress modulators for the treatment of disease)

IT Biological transport

(export; nitrosative and oxidative stress modulators for the treatment of disease)

```
Antitumor agents
ΙT
     Antitumor agents
        (head carcinoma; nitrosative and oxidative stress modulators for the
        treatment of disease)
IT
     Mouth
     Mouth
        (infection; nitrosative and oxidative stress modulators for the
        treatment of disease)
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     X-ray
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IT
     Skin, disease
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        of disease)
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IT
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ΙT
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        (melanoma; nitrosative and oxidative stress modulators for the
        treatment of disease).
     Antitumor agents
IT
     Antitumor agents
        (neck carcinoma; nitrosative and oxidative stress modulators for the
        treatment of disease)
IT
     Nitrosation
        (nitrosating agents; nitrosative and oxidative stress modulators for
        the treatment of disease)
IΤ
     Alkylating agents, biological
     Anthelmintics
     Antibacterial agents
     Antihypotensives
                                    Committee the second second
     Antimicrobial agents
     Antitumor agents
     Antiviral agents
     Chemotherapy
     Cytotoxic agents
     Drug resistance
     Escherichia coli
     Fungicides
     Genetic vectors
     Immune system
     Oxidative stress, biological
     Protozoacides
     Psoriasis
     Radiotherapy
        (nitrosative and oxidative stress modulators for the treatment of
        disease)
ΙT
     Acids, biological studies
     Chelating agents
     Cytokines
```

TΤ

IT

ΙT

Nitrates, biological studies Nitrites RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (nitrosative and oxidative stress modulators for the treatment of disease) Stress, animal Stress, microbial (nitrosative; nitrosative and oxidative stress modulators for the treatment of disease) Peptides, biological studies RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (nitrosylated; nitrosative and oxidative stress modulators for the treatment of disease) Gene, microbial ΙT RL: BSU (Biological study, unclassified); BIOL (Biological study) (oxyR; nitrosative and oxidative stress modulators for the treatment of disease) IT Proliferation inhibition (proliferation inhibitors; nitrosative and oxidative stress modulators for the treatment of disease) Disease, animal (proliferative, myoproliferative disorders; nitrosative and oxidative stress modulators for the treatment of disease) ΙT Catalysts (redox active metal catalysts; nitrosative and oxidative stress modulators for the treatment of disease) IT Artery, disease (restenosis; nitrosative and oxidative stress modulators for the treatment of disease) ΙT Antitumor agents Antitumor agents Antitumor agents (small intestine, metastasis, from melanoma; nitrosative and oxidative stress modulators for the treatment of disease) ΙT Intestine, neoplasm Intestine, neoplasm - 11 Intestine, neoplasm (small, inhibitors, metastasis, from melanoma; nitrosative and oxidative stress modulators for the treatment of disease) IT Lung, neoplasm (small-cell carcinoma, inhibitors; nitrosative and oxidative stress modulators for the treatment of disease) ΙT Polymers, biological studies RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses) (stent coated with; nitrosative and oxidative stress modulators for the treatment of disease) IT Medical goods (stents; nitrosative and oxidative stress modulators for the treatment of disease) ΙT Brain, disease (stroke; nitrosative and oxidative stress modulators for the treatment of disease) ΙT P-glycoproteins RL: BSU (Biological study, unclassified); BIOL (Biological study)

for the treatment of disease)

(substrates and inhibitors; nitrosative and oxidative stress modulators

```
IT
     Sulfites
     RL: BSU (Biological study, unclassified); BIOL (Biological study)
        (sulfite-metabolizing enzymes; nitrosative and oxidative stress
       modulators for the treatment of disease)
IT
     Enzymes, biological studies
     RL: BAC (Biological activity or effector, except adverse); BSU (Biological
     study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES
     (Uses)
        (sulfite-metabolizing; nitrosative and oxidative stress modulators for
        the treatment of disease)
IT
     51209-75-7, S-Nitrosocysteine
     RL: BAC (Biological activity or effector, except adverse); BSU (Biological
     study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES
     (Uses)
        (and S-Nitrosocysteine-containing tripeptides; nitrosative and oxidative
        stress modulators for the treatment of disease)
TΤ
     50-18-0, Cyclophosphamide 57-22-7, Vincristine
     RL: BAC (Biological activity or effector, except adverse); BSU (Biological
     study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES
     (Uses)
        (combination therapy; nitrosative and oxidative stress modulators for
        the treatment of disease)
IT
     9054-75-5, Guanylyl cyclase
     RL: BSU (Biological study, unclassified); BIOL (Biological study)
        (inhibitors; nitrosative and oxidative stress modulators for the
        treatment of disease)
     12587-47-2, \beta-Particle
ΙT
     RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
        (irradiation; nitrosative and oxidative stress modulators for the treatment
        of disease)
     113158-67-1D, L-Buthionine-S-sulfoximine, NO-substituted
ΙT
     RL: BAC (Biological activity or effector, except adverse); BSU (Biological
     study, unclassified); DEV (Device component use); THU (Therapeutic use);
     BIOL (Biological study); USES (Uses)
        (nitrosative and oxidative stress modulators for the treatment of
        disease)
IT
     204438-84-6P
     RL: BAC (Biological activity or effector, except adverse); BSU (Biological
     study, unclassified); SPN (Synthetic preparation); THU (Therapeutic
     use); BIOL (Biological study); PREP (Preparation); USES (Uses)
        (nitrosative and oxidative stress modulators for the treatment of
        disease)
IT
                                         54-85-3D, Isoniazid, NO-substituted
     52-53-9D, Verapamil, NO-substituted
     127-07-1, Hydroxyurea 148-82-3, Melphalan 13292-46-1D, Rifampin,
                      23214-92-8D, Doxorubicin, NO-substituted
     NO-substituted
                                                                 32467-88-2
     113158-67-1, L-Buthionine-S-sulfoximine
                                              139427-42-2 204438-79-9
     204438-80-2
                 204438-81-3 204438-82-4
                                               204438-83-5
     RL: BAC (Biological activity or effector, except adverse); BSU (Biological
     study, unclassified); THU (Therapeutic use); BIOL (Biological
     study); USES (Uses)
        (nitrosative and oxidative stress modulators for the treatment of
        disease)
IT
     70-18-8, Glutathione, biological studies
                                                6027-13-0, L-Homocysteine
     9023-64-7, \gamma-Glutamylcysteine synthetase
                                                10102-43-9, Nitric oxide,
     biological studies 14452-93-8, Nitrosyl ion
                                                    14797-65-0, Nitrite,
     biological studies
                          14967-78-3
     RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL
     (Biological study); PROC (Process)
        (nitrosative and oxidative stress modulators for the treatment of
        disease)
```

- IT 109-79-5, 1-Butanethiol
  - RL: RCT (Reactant); RACT (Reactant or reagent)
     (reaction; nitrosative and oxidative stress modulators for the
     treatment of disease)
- IT 9013-03-0, Nitrate reductase 9080-03-9, Nitrite reductase RL: BSU (Biological study, unclassified); BIOL (Biological study) (substrates; nitrosative and oxidative stress modulators for the treatment of disease)
- RE.CNT 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS RECORD RE
- (1) Abrams; US 5112954 A 1992 HCAPLUS
- (2) Anderson; US 5476966 A 1995 HCAPLUS
- (3) Andrew, P; Biochemical and Biophysical Research Communications 1995, V214(3), P949 HCAPLUS
- (4) Baldwin; US 4666835 A 1987 HCAPLUS
- (5) Benet; US 5567592 A 1996 HCAPLUS
- (6) Bogle, R; British Journal of Pharmacology 1992, V105, P768 HCAPLUS
- (7) Bounous; US 5290571 A 1994 HCAPLUS
- (8) Carter; US 5362309 A 1994
- (9) Cook; US 5578718 A 1996 HCAPLUS
- (10) Crosson; US 4966577 A 1990
- (11) Debelder, A; The Lancet 1995, V345, P124 MEDLINE
- (12) Degroote, M; Science 1996, V272, P414 HCAPLUS
- (13) Griffith; US 5294736 A 1994 HCAPLUS
- (14) Guillemard, E; Antimicrobial Agents and Chemotherapy 1996, V40(4), P1057 HCAPLUS
- (15) Hara; US 5316767 A 1994 HCAPLUS
- (16) Hausladen, A; Cell 1996, V86(5), P719 HCAPLUS
- (17) Held, K; Mutation Research 1993, V299, P261 HCAPLUS
- (18) Iversen; US 5641754 A 1997 HCAPLUS
- (19) Kitahara; US 4927808 A 1990 HCAPLUS
- (20) Kronenthal; US 5616775 A 1997 HCAPLUS
- (21) Martani; US 4834965 A 1989 HCAPLUS
- (22) Mebmer, U; FEBS Letters 1994, V355, P23
- (23) Moore, W; Proceedings of the National Academy of Science 1989, V86, P1461 HCAPLUS
- (24) Mueller; US 5342853 A 1994 HCAPLUS - - -
- (25) Radomski, M; British Journal of Pharmacologyl 1992, V107, P745 HCAPLUS
- (26) Ramsey, B; British Journal of Clinical Pathology 1995, V40, P101
- (27) Shapiro; US 4898878 A 1990 HCAPLUS
- (28) Shapland; US 5286254 A 1994
- (29) Shapland; US 5628730 A 1997
- (30) Singh, R; The Journal of Biological Chemistry 1996, V271(31), P18596 HCAPLUS
- (31) Stamler; US 5385937 A 1995 HCAPLUS
- (32) Stamler; US 5593876 A 1997 HCAPLUS
- (33) Struck, A; FEBS Letters 1995, V361, P291 HCAPLUS
- (34) Suli; US 4950651 A 1990 HCAPLUS
- (35) Wang, T; Cellular Pharmacology 1995, V2, P237 HCAPLUS
- (36) Wink, D; The Journal of Biological Chemistry 1997, V272(17), P11147 HCAPLUS
- (37) Witzel; US 5639741 A 1997 HCAPLUS
- (38) Yi-Zun, J; Chinese Medical Journal 1992, V105(8), P647
- (39) Young, D; Annual Review of Microbiology 1995, V49, P641 HCAPLUS
- IT 204438-84-6P
  - RL: BAC (Biological activity or effector, except adverse); BSU (Biological

study, unclassified); SPN (Synthetic preparation); THU (Therapeutic
use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (nitrosative and oxidative stress modulators for the treatment of
 disease)

RN 204438-84-6 HCAPLUS

CN Butanoic acid, 2-amino-4-(S-butylsulfonimidoyl)-2-ethyl- (9CI) (CA INDEX NAME)

IT 204438-79-9

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(nitrosative and oxidative stress modulators for the treatment of disease)

RN 204438-79-9 HCAPLUS

CN Butanoic acid, 2-amino-4-(S-butylsulfonimidoyl)-2-ethyl-, [S-(R\*,R\*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L33 ANSWER 3 OF 9 HCAPLUS COPYRIGHT 2006 ACS on STN

AN 1990:32528 HCAPLUS

DN 112:32528

ED Entered STN: 04 Feb. 1990ter

TI Inhibition of Escherichia coli glutamine synthetase by  $\alpha-$  and  $\gamma-substituted phosphinothricins$ 

AU Logusch, Eugene W.; Walker, Daniel M.; McDonald, John F.; Franz, John E.; Villafranca, Joseph J.; DiIanni, Carolyn L.; Colanduoni, John A.; Li, Bin; Schineller, Jeffrey B.

CS Monsanto Agric. Co., St. Louis, MO, 63198, USA

SO Biochemistry (1990), 29(2), 366-72 CODEN: BICHAW; ISSN: 0006-2960

DT Journal

LA English

CC 7-3 (Enzymes)

The inhibition of E. coli glutamine synthetase (GS) with  $\alpha$ - and  $\gamma$ -substituted analogs of phosphinothricin [L-2-amino-4-(hydroxymethylphosphinyl)butanoic acid (PPT)], a naturally occurring inhibitor of GS, was investigated. These compds. displayed inhibition of bacterial GS that was competitive vs. L-glutamate, with Ki values in the low micromolar range. At concns. greater than Ki, the phosphinothricins caused time-dependent loss of enzyme activity, whereas dilution after enzyme inactivation resulted in recovery of enzyme activity.

ATP was required for inactivation; the nonhydrolyzable ATP analog, AMP-PCP, failed to support inhibition of GS by the phosphinothricins. binding of these inhibitors to the enzyme was also characterized by measurement of changes in protein fluorescence, which provided similar inactivation rate consts., k1 and k2, for the entire series of compds. Rate consts. (koff) for recovery were also determined by fluorescence measurement and were comparable for both PPT and the  $\gamma\text{-hydroxylated}$ analog, DL-γ-hydroxyphosphinothricin (GHPPT), and significantly greater for the  $\alpha-$  and  $\gamma-$ alkyl-substituted compds. EPR spectra provided information on the interaction of the phosphinothricins with the Mn form of the enzyme in the absence of ATP, and significant binding was observed for PPT and GHPPT. 31P NMR expts. confirmed that enzyme inactivation was accompanied by hydrolysis of ATP, although phosphorylated phosphinothricins could not be detected in solution The kinetic behavior of these compds. was consistent with a mechanism involving inhibitor phosphorylation, followed by release from the active site and simultaneous hydrolysis to form phosphate and free inhibitor.

ST glutamine synthetase inhibition phosphinothricin deriv Escherichia

IT Escherichia coli

(glutamine synthetase of, inhibition of, by phosphinothricin derivs., kinetics and mechanism of)

IT Kinetics, enzymic

(of inhibition, of glutamine synthetase of Escherichia coli, by phosphinothricin derivs.)

IT 51276-47-2, DL-Phosphinothricin **115730-43-3** 119567-65-6

119617-93-5 119617-94-6 121249-46-5

RL: BIOL (Biological study)

(glutamine synthetase of Escherichia coli inhibition by, kinetics and mechanism of)

IT 9023-70-5, Glutamine synthetase

RL: BIOL (Biological study)

(inhibition of, of Escherichia coli, by phosphinothricin derivs., kinetics and mechanism of)

IT 115730-43-3

RL: BIOL (Biological study)

(glutamine synthetase of Escherichia coli inhibition by, kinetics and mechanism of)

RN 115730-43-3 HCAPLUS

CN Isovaline, 4-(hydroxymethylphosphinyl)-, monoammonium salt (9CI) (CA INDEX NAME)

## ● инз

#### IT 9023-70-5, Glutamine synthetase

RL: BIOL (Biological study)

(inhibition of, of Escherichia coli, by phosphinothricin derivs., kinetics and mechanism of)

RN 9023-70-5 HCAPLUS

CN Synthetase, glutamine (9CI) (CA INDEX NAME)

```
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
L33
    ANSWER 4 OF 9 HCAPLUS COPYRIGHT 2006 ACS on STN
AN
     1989:150325 HCAPLUS
DN
     110:150325
ED
     Entered STN: 30 Apr 1989
ΤI
     Substrate variability as a factor in enzyme inhibitor design: inhibition
     of ovine brain glutamine synthetase by \alpha- and
     γ-substituted phosphinothricins
ΑU
     Logusch, Eugene W.; Walker, Daniel M.; McDonald, John F.; Franz, John E.
CS
     Monsanto Agric. Co., Unit Monsanto Co., St. Louis, MO, 63198, USA
SO
     Biochemistry (1989), 28(7), 3043-51
     CODEN: BICHAW; ISSN: 0006-2960
DT
     Journal
LA
     English
CC
     7-3 (Enzymes)
AB
     Ovine brain glutamine synthetase (GS) utilizes various
     substituted glutamic acids as substrates. This information was used to
     design \alpha- and \gamma-substituted analogs of phosphinothricin
     [L-2-amino-4-(hydroxymethylphosphinyl)butanoic acid, PPT], a naturally
     occurring inhibitor of GS. These compds. displayed competitive inhibition
     of GS, and a correlation between the inhibitor Ki values and the Km/Vmax
     values of the analogously substituted glutamates supports the hypothesis
     that the phosphinothricins participate in transition-state analog
     inhibition of GS. At concns. >Ki, these inhibitors caused biphasic
     time-dependent loss of enzyme activity, with initial pseudo-1st-order
     behavior; k'inact parameters were determined for several compds. and were
     similar to the 2.1 + 10-2 s-1 value measured for PPT. Dilution after
     GS inactivation caused a non-1st-order recovery of activity. Reactivation
     kinetics were insensitive to inhibitor and ADP concns. over wide ranges,
     although very high postdiln. concns. of inhibitor suppressed reactivation.
     The burst activity level, \beta, as well as the concentration of inhibitor
     required to suppress reactivation to this level, \mu, expressed as a
     multiple of the Ki value, was characteristic for each compound in the
     phosphinothricin series. Increasing substitution of the phosphinothricin
     parent structure caused an increase in Ki values as well as in the
     inactivation/reactivation parameters. The kinetic behavior of these
     inhibitors was consistent with a mechanistic scheme involving initial
     phosphorylation and rapid partial inhibitor dissociation, followed by slow
     release of remaining bound inhibitor.
ST
     brain glutamine synthetase inhibition phosphinothricin
     analog
IT
     Brain, composition
        (glutamine synthetase of, inhibition of, by
        phosphinothricin analogs)
IT
     Kinetics, enzymic
        (of inhibition of, of glutamine synthetase of
        brain, by phosphinothricin analogs)
IT
     Molecular structure-biological activity relationship
        (glutamine synthetase-inhibiting, of
        phosphinothricin analogs)
IT
    ·21752-32-9
                  51276-47-2 115730-43-3 119567-65-6 119567-66-7
     119617-93-5
                   119617-94-6
     RL: BIOL (Biological study)
        (glutamine synthetase of brain inhibition by,
        kinetics of, structure in relation to)
     9023-70-5, Glutamine synthetase
IT
     RL: PROC (Process)
        (inhibition of, of brain, by phosphinothricin analogs, structure in
```

relation to)

IT 115730-43-3

RL: BIOL (Biological study)

(glutamine synthetase of brain inhibition by,

kinetics of, structure in relation to)

RN 115730-43-3 HCAPLUS

CN Isovaline, 4-(hydroxymethylphosphinyl)-, monoammonium salt (9CI) (CA INDEX NAME)

NH3

IT 9023-70-5, Glutamine synthetase

RL: PROC (Process)

(inhibition of, of brain, by phosphinothricin analogs, structure in

1. "\$P\$不好。" 2. 沙特

relation to)

RN 9023-70-5 HCAPLUS

CN Synthetase, glutamine (9CI) (CA INDEX NAME)

\*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*

L33 ANSWER 5 OF 9 HCAPLUS COPYRIGHT 2006 ACS on STN

AN 1988:510882 HCAPLUS

DN 109:110882

ED Entered STN: 01 Oct 1988

TI Synthesis of  $\alpha$ - and  $\gamma$ -alkyl-substituted phosphinothricins:

potent new inhibitors of glutamine synthetase

AU Logusch, Eugene W.; Walker, Daniel M.; McDonald, John F.; Leo, Gregory C.; Franz, John E.

CS Monsanto Agric. Co., St. Louis, MO, 63167, USA

SO Journal of Organic Chemistry (1988), 53(17), 4069-74

CODEN: JOCEAH; ISSN: 0022-3263

DT Journal

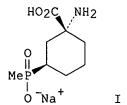
LA English

CC 34-2 (Amino Acids, Peptides, and Proteins)

Section cross-reference(s): 7, 29

OS CASREACT 109:110882

GI



AB Considerations of substrate structural variability for the enzyme

1155.47 强高

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glutamine synthetase (GS, E.C. 6.3.1.2) have led to the
     design of \alpha- and \gamma-substituted analogs of the naturally
     occurring GS inhibitor phosphinothricin (PPT). The novel cyclic inhibitor
     DL-cyclohexanephosphinothricin (I) was prepared via conjugate addition of
     MeP(OEt)2 to 2-cyclohexenone, followed by stereospecific Bucherer-Bergs
     amino acid synthesis. The stereochem. of I was determined by 2-dimensional NMR
     techniques. The substitute phosphinothricins function as active site
     probes useful for elucidating the mechanism of GS inhibition by PPT.
     cyclohexanephosphinotricin prepn glutamine synthetase
ST
     inhibitor; phosphinotricin analog prepn glutamine
     synthetase inhibitor; Bucherer Bergs phosphinocyclohexanone
IT
     586-75-4, p-Bromobenzoyl chloride
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (amidation of, with amino(phosphono)cyclohexanecarboxylate)
     9023-70-5, Glutamine synthetase
IT
     RL: PROC (Process)
        (inhibition of, with phosphinothricin analogs)
IT
     115651-56-4P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (preparation and acylation of, with bromobenzoyl chloride)
     73870-64-1P
                  86605-52-9P 115651-42-8P 115651-51-9P
TΤ
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (preparation and cyclocondensation reaction of, with ammonium carbonate and
        potassium cyanide)
IT
     115651-53-1P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (preparation and esterification of, with diazomethane)
     35597-44-5DP, Phosphinothricin, analogs 115651-45-1P
TΤ
                  115651-54-2P 115730-43-3P
     115651-49-5P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (preparation and glutamine synthetase-inhibiting
        activity of)
                   115651-40-6P
IT
                                 115651-41-7P
                                                 115651-50-8P
     86605-51-8P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (preparation and hydrolysis of)
TΤ
     86605-54-1P
                   115651-43-9P 115651-44-0P
                                                 115651-52-0P
     RL: RCT (Reactant); SPN=(Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (preparation and saponification of, with barium hydroxide)
TΤ
     115651-46-2P
                   115651-47-3P 115651-48-4P 115651-55-3P
                                                                 115651-57-5P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (preparation of)
TΤ
     78-94-4, Methyl vinyl ketone, reactions 930-68-7, 2-Cyclohexenone
     1629-58-9, Ethyl vinyl ketone 4170-30-3, Croton aldehyde
                                                                 16205-98-4
     115651-58-6
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (reaction of, with di-Et Me phosphinate)
IT
     15715-41-0
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (reaction of, with unsatd. aldehydes and ketones)
ΙT
     9023-70-5, Glutamine synthetase
     RL: PROC (Process)
        (inhibition of, with phosphinothricin analogs)
RN
     9023-70-5 HCAPLUS
CN
     Synthetase, glutamine (9CI) (CA INDEX NAME)
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\*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*

IT 115651-45-1P 115730-43-3P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation and glutamine synthetase-inhibiting
 activity of)

RN 115651-45-1 HCAPLUS

CN Butanoic acid, 2-amino-2-ethyl-4-(hydroxymethylphosphinyl)-, monosodium salt (9CI) (CA INDEX NAME)

Na

RN 115730-43-3 HCAPLUS

CN Isovaline, 4-(hydroxymethylphosphinyl)-, monoammonium salt (9CI) (CA
INDEX NAME)

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NH3

L33 ANSWER 6 OF 9 HCAPLUS COPYRIGHT 2006 ACS on STN

AN 1988:132274 HCAPLUS

DN 108:132274 - 10 1202 7 10 1202

ED Entered STN: 15 Apr 1988

TI Amino acid sulfoximines:  $\alpha$ -ethylmethionine sulfoximine

AU Griffith, Owen W.

CS Med. Coll., Cornell Univ., New York, NY, 10021, USA

SO Methods in Enzymology (1987), 143(Sulfur Sulfur Amino Acids), 286-91

CODEN: MENZAU; ISSN: 0076-6879

DT Journal

LA English

CC 34-2 (Amino Acids, Peptides, and Proteins)

AB  $\alpha$ -Ethylmethionine sulfoxime, HO2CCEt(NH2)CH2CH2S(O)Me:NH, was prepared by treatment of HO2CCEt(NH2)CH2CH2SMe (I) with HCl. I was prepared by treatment of EtCOCH:CH2 with MeSH to give EtCOCH2CH2SMe which was converted to a hydantoin derivative with (NH4)2CO3 and NaCN and the product hydrolyzed to I.

ST ethylmethionine sulfoximine

IT 66735-70-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

the and laboration to

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issac - 10 / 715679
        (preparation and hydrolysis of)
IT
     66735-71-5P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (preparation and reaction with hydrazoic acid)
IT
     66735-68-0P
                   113350-10-0P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (preparation of)
     66735-69-1P, Ethyl 2-(methylthio)ethyl ketone
IT
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (preparation of and hydantoin derivative preparation from)
TΤ
     74-93-1, Methanethiol, reactions
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (reaction of, with Et vinyl ketone)
ΙT
     7782-79-8, Hydrazoic acid
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (reaction of, with ethylmethionine)
IT
     1629-58-9, Ethyl vinyl ketone
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (reaction of, with methanethiol)
ΙT
     66735-68-0P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (preparation of)
RN
     66735-68-0 HCAPLUS
CN
     Butanoic acid, 2-amino-2-ethyl-4-(S-methylsulfonimidoyl)- (9CI) (CA INDEX
   NH2
Et-C-CH_2-CH_2-S-Me
   CO2H
L33 ANSWER 7 OF 9 HCAPLUS COPYRIGHT 2006 ACS on STN
AN
     1981:457044 HCAPLUS
DN
     95:57044
ED
     Entered STN: 12 May 1984
TI
     Inhibition of rat liver glutamine synthetase by
     phosphonic analogs of glutamic acid
     Lejczak, B.; Starzemska, H.; Mastalerz, P.
ΑU
CS
     Inst. Org. Phys. Chem., Tech. Univ., Wroclaw, PL-50370, Pol.
SO
     Experientia (1981), 37(5), 461-2
     CODEN: EXPEAM; ISSN: 0014-4754
DT
     Journal
     English
LA
```

L-glutamate.

ST glutamine synthetase inhibition glutamate analog; phosphonate analog glutamate glutamine synthetase inhibition

IT Liver, composition

7-3 (Enzymes)

synthetase.

CC

AΒ

(glutamine synthetase of, phosphoric analogs of glutamate inhibition of)

which the  $\alpha$ - or  $\gamma$ -COOH groups are replaced by PO3H2 or

The Ki values are comparable to or lower than Km for

Analogs of glutamic acid,  $\alpha$ -methylglutamic acid, and glutamine in

P(O)(OH3)OH groups competitively inhibit rat liver glutamine

```
IT
     Michaelis constant
        (of glutamine synthetase)
     Kinetics, enzymic
ΙT
        (of inhibition, of glutamine synthetase)
IT
     Molecular structure-biological activity relationship
        (glutamine synthetase-inhibiting, of glutamate
        phosphonic analogs)
     56-85-9D, phosphonic analogs 56-86-0D, phosphonic analogs
IT
                                                                   6323-99-5
     18865-31-1
                  51276-47-2 65482-86-2 73870-68-5 73870-69-6
     78405-44-4
                  78405-48-8 78432-42-5 81746-56-7 115692-97-2
     153605-27-7
     RL: BIOL (Biological study)
        (glutamine synthetase inhibition by)
ΙT
     9023-70-5
     RL: PROC (Process)
        (inhibition of, by phosphonic analogs of glutamic acid)
IT
     65482-86-2 78405-44-4
     RL: BIOL (Biological study)
        (glutamine synthetase inhibition by)
RN
     65482-86-2 HCAPLUS
CN
     Isovaline, 4-(hydroxymethylphosphinyl)- (9CI) (CA INDEX NAME)
        CH2-CH2
                 OH
     Me
RN
     78405-44-4 HCAPLUS
CN
     Isovaline, 4-phosphono- (9CI) (CA INDEX NAME)
HO2C
IT ....9023-70-5
                                                                              True winger of the
     RL: PROC (Process)
        (inhibition of, by phosphonic analogs of glutamic acid)
RN
     9023-70-5 HCAPLUS
CN
     Synthetase, glutamine (9CI) (CA INDEX NAME)
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
L33
    ANSWER 8 OF 9 HCAPLUS COPYRIGHT 2006 ACS on STN
AN
     1979:198299 HCAPLUS
DN
     90:198299
ED
     Entered STN: 12 May 1984
     Inhibition of glutathione biosynthesis by prothionine sulfoximine
TΤ
     (S-n-propyl homocysteine sulfoximine), a selective inhibitor of
     \gamma-glutamylcysteine synthetase
     Griffith, Owen W.; Anderson, Mary E.; Meister, Alton
ΑU
CS
     Med. Coll., Cornell Univ., New York, NY, USA
     Journal of Biological Chemistry (1979), 254(4), 1205-10
SO
     CODEN: JBCHA3; ISSN: 0021-9258
```

DT

Journal

```
LA
     English
CC
     3-5 (Biochemical Interactions)
     Section cross-reference(s): 7
AB
     DL-Prothionine SR-sulfoximine [70085-86-8] and \alpha-methyl-DL-
     prothionine-SR-sulfoximine [70056-05-2] were prepared and found
     to markedly inhibit \gamma-glutamylcysteine synthetase [9023-64-7] but
     to not significantly affect glutamine synthetase [
     9023-70-5]. After injection of prothionine sulfoximine into mice,
     the level of kidney glutathione [70-18-8] decreased rapidly to .apprx.20%
     of the control level indicating that a large fraction, rather than a small
     pool, of glutathione participates in rapid turnover. The rapid decline of
     the glutathione level that occurs after inhibition of glutathione
     synthesis reflects the normal rate of intracellular glutathione
     utilization by the \gamma-glutamyl cycle. A number of related sulfoximines
     were synthesized and tested as inhibitors of glutamine and
     \gamma-glutamylcysteine synthetases.
ST
     glutathione formation prothionine sulfoximine; glutamylcysteine synthetase
     prothionine sulfoximine
     Kidney, metabolismit to have a more
TΤ
         (glutathione formation by, prothionine sulfoximine inhibition of)
IT
     Molecular structure-biological activity relationship
         (glutamylcysteine synthetase-inhibiting, of prothionine sulfoximine
        analogs)
ΙT
     70-18-8, biological studies
     RL: FORM (Formation, nonpreparative)
         (formation of, by kidney, methionine sulfoximine inhibition of)
IT
     15985-39-4 66735-67-9 66735-68-0
     RL: PRP (Properties)
         (glutamylcysteine synthetase inhibition by)
IT
     9023-64-7
     RL: PROC (Process)
         (methionine sulfoximine inhibition of)
                                  70056-01-8P
                                                70056-02-9P 70056-03-0P
TΤ
     15985-39-4P
                   70056-00-7P
                                  70085-87-9P
     70056-05-2P
                   70085-86-8P
     RL: PREP (Preparation)
         (preparation and glutamylcysteine synthetase-inhibiting activity of)
IT
     44768-66-3P
     RL: SPN (Synthetic preparation); PREP (Preparation)
         (preparation and hydantoinylation of)
     70085-85-7P
1000 RED RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RAGT電路可能等 1000 PREP
     (Reactant or reagent)
         (preparation and saponification of)
     557-02-8P. 2598-46-1P 2749-07-7P 16820-52-3P
IT
                                                          16820-66-9P
     42537-72-4P
                   70056-04-1P 70056-06-3P 70095-14-6P
     RL: PREP (Preparation)
         (preparation of)
IT
     9023-70-5
     RL: PRP (Properties)
         (prothionine sulfoximine inhibition of glutamylcysteine synthetase in
        relation to)
     107-03-9
ΙT
     RL: RCT (Reactant); RACT (Reactant or reagent)
         (reaction of, with acrolein)
IT
     107-02-8, biological studies
     RL: RCT (Reactant); RACT (Reactant or reagent)
         (reaction of, with propanethiol)
ΙT
     14109-74-1
     RL: RCT (Reactant); RACT (Reactant or reagent)
         (reductive amination of)
```

IT 66735-67-9 66735-68-0

RL: PRP (Properties)

(glutamylcysteine synthetase inhibition by)

大路流水机,减速加

RN 66735-67-9 HCAPLUS

CN Isovaline, 4-(S-methylsulfonimidoyl)- (9CI) (CA INDEX NAME)

RN 66735-68-0 HCAPLUS

CN Butanoic acid, 2-amino-2-ethyl-4-(S-methylsulfonimidoyl)- (9CI) (CA INDEX NAME)

IT 70056-03-0P 70056-05-2P

RL: PREP (Preparation)

(preparation and glutamylcysteine synthetase-inhibiting activity of)

RN 70056-03-0 HCAPLUS

CN Isovaline, 4-(S-ethylsulfonimidoyl)- (9CI) (CA INDEX NAME)

A MARKO 1880 - WAS RN 70056-05-2 HCAPLUS

CN Isovaline, 4-(S-propylsulfonimidoyl)- (9CI) (CA INDEX NAME)

IT 9023-70-5

RL: PRP (Properties)

(prothionine sulfoximine inhibition of glutamylcysteine synthetase in relation to)

RN 9023-70-5 HCAPLUS

CN Synthetase, glutamine (9CI) (CA INDEX NAME)